Piperazine 110-85-0 | DTXSID1021164

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 5.37 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.36e-01

Confidence level: 7.13e-01

Nearest Neighbors from the Training Set

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Piperazine Measured: 11.6 Predicted: 5.37

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Piperazine dihydrochloride

Measured: 2.58 Predicted: 5.37

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2-Methylpiperazine Measured: 4.34 Predicted: 4.68

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2-Methylpyrazine Measured: 10.6 Predicted: 4.35